Physics-Informed Neural Networks (PINNs)

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Overview

Outline

Learning Objectives

- Understand why standard neural networks fail for physics problems
- Learn how to incorporate physics into neural network training
- Master automatic differentiation for computing derivatives
- Compare data-driven vs physics-informed approaches

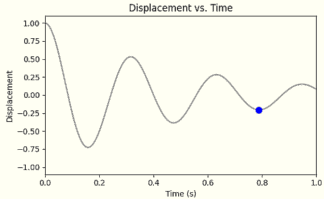
▸ Open Notebook: PINN

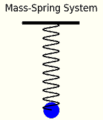
The Problem: A Damped Harmonic Oscillator

A mass m on a spring (constant k) with damping (coefficient c). The displacement $u(t)$ satisfies:

$$m\frac{d^2u}{dt^2} + c\frac{du}{dt} + ku = 0$$

with initial conditions: $u(0) = 1$, $\frac{du}{dt}(0) = 0$.





A classic physics problem to illustrate PINNs.

The Challenge: Reconstruct the full solution $u(t)$ from a few sparse, noisy data points.

Stage 1: The Data-Only Approach

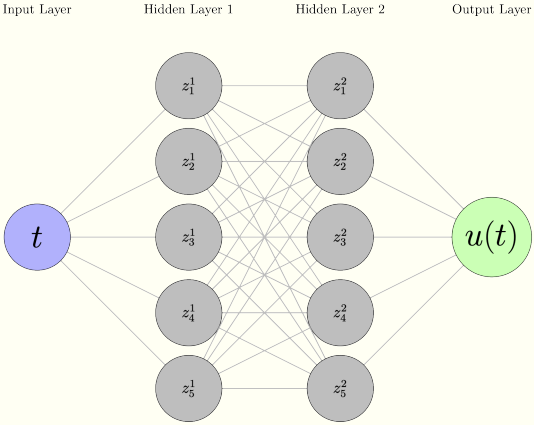
Idea: Train a standard neural network to fit the sparse data.

Loss Function: Mean Squared Error

$$\mathcal{L}_{\text{data}}(\theta) = \frac{1}{N} \sum_{i=1}^{N} |\hat{u}_\theta(t_i) - u_i|^2$$

Architecture:

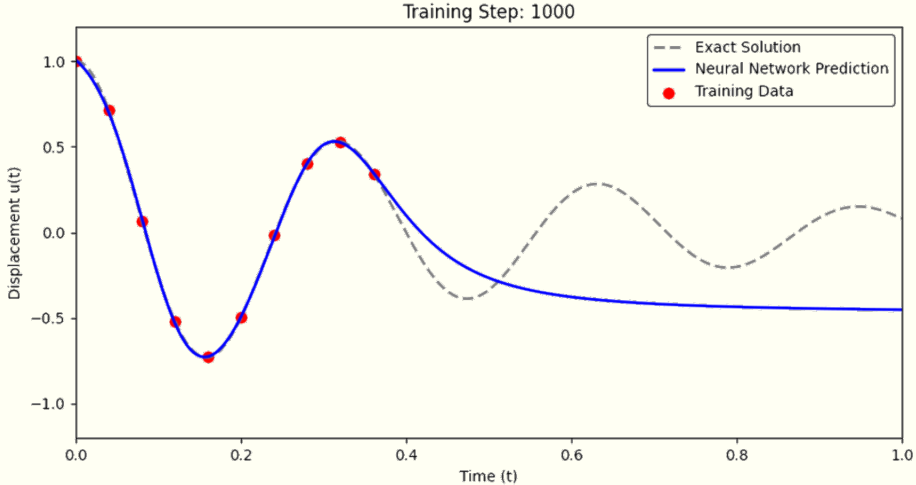
- Input: Time t
- Hidden Layers: Tanh activations
- Output: Displacement $\hat{u}_\theta(t)$



Standard NN for function fitting.

The Failure of the Data-Only Approach

Result: The network fits the training points but fails catastrophically between them.



The network overfits to the sparse data and does not respect the underlying physics

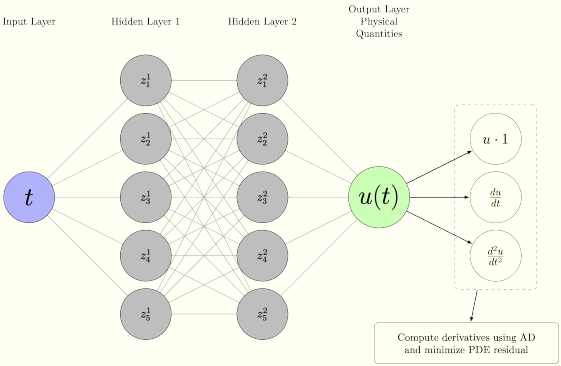
Stage 2: Enter Physics-Informed Neural Networks

The Key Insight: Don't just fit data. Enforce the differential equation itself!

Physics Residual: We define a residual based on the ODE:

$$\mathcal{R}_\theta(t) = m\frac{d^2\hat{u}_\theta}{dt^2} + c\frac{d\hat{u}_\theta}{dt} + k\hat{u}_\theta$$

If the solution is correct, $\mathcal{R}_\theta(t)$ should be zero.



PINN architecture with physics loss.

The Complete PINN Loss Function

The total loss is a combination of data fit and physics enforcement.

$$\mathcal{L}_{\text{total}}(\theta) = \mathcal{L}_{\text{data}}(\theta) + \lambda \mathcal{L}_{\text{physics}}(\theta)$$

Data Loss

Ensures the solution passes through the measurements.

$$\mathcal{L}_{\text{data}}(\theta) = \frac{1}{N_{\text{data}}} \sum_{i=1}^{N_{\text{data}}} |\hat{u}_\theta(t_i) - u_i|^2$$

Physics Loss

Ensures the solution obeys the ODE at random "collocation" points.

$$\mathcal{L}_{\text{physics}}(\theta) = \frac{1}{N_{\text{colloc}}} \sum_{j=1}^{N_{\text{colloc}}} |\mathcal{R}_\theta(t_j)|^2$$

The Secret Weapon: Automatic Differentiation (AD)

Critical Question: How do we compute $\frac{d\hat{u}_\theta}{dt}$ and $\frac{d^2\hat{u}_\theta}{dt^2}$?

Answer: Automatic Differentiation

AD provides **exact** derivatives of the neural network output with respect to its input, by applying the chain rule through the computational graph.

- No finite difference errors.
- Computationally efficient (especially reverse-mode AD).
- Built into modern frameworks (PyTorch, TensorFlow, JAX).

Example: For $u(t) = \sin(t)$, AD can compute $u'(t) = \cos(t)$ and $u''(t) = -\sin(t)$ to machine precision.

Theoretical Foundation: UAT for Sobolev Spaces

Classical UAT: NNs can approximate any *continuous function*.
Problem: For PDEs, we need to approximate functions **and their derivatives**.

Extended Universal Approximation Theorem

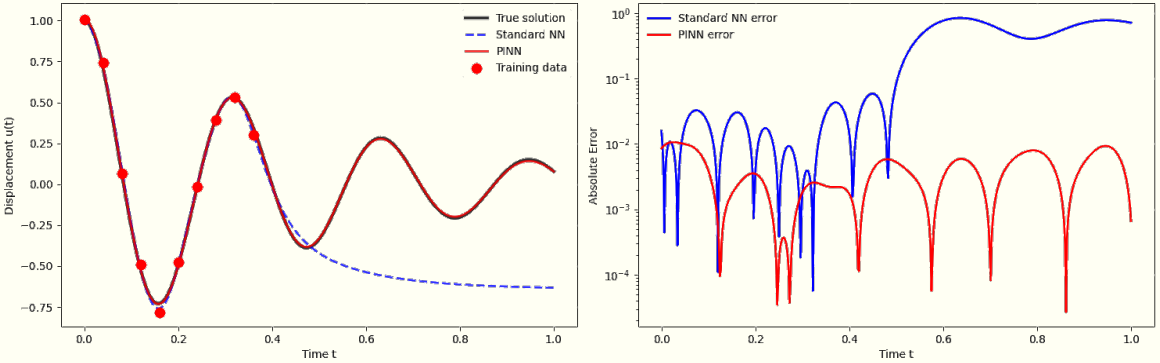
Neural networks with sufficiently smooth activation functions (e.g., tanh, not ReLU) can approximate functions in **Sobolev spaces** $H^k(\Omega)$.

$$\|u - \hat{u}_\theta\|_{H^k} < \epsilon$$

The Sobolev norm $\|u\|_{H^k}^2 = \sum_{|\alpha| \leq k} \|D^\alpha u\|_{L^2}^2$ measures the error in the function and all its derivatives up to order k.

Why this matters: For a k^{th}-order ODE/PDE, we need an activation function that is at least k times differentiable (C^k). For our 2nd-order oscillator, we need a C^2 activation like tanh.

The Moment of Truth: Standard NN vs. PINN



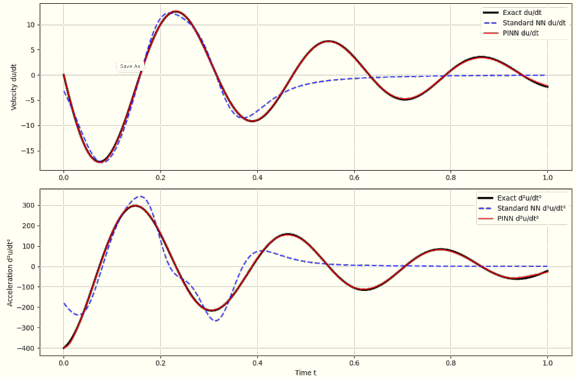
Placeholder for the comparison plot from the notebook.

Observation:

- **Standard NN:** Fits data points, but fails to generalize.
- **PINN:** Fits data points AND follows the physics, resulting in a globally accurate solution.

Deep Dive: Derivative and Phase Portrait Analysis

The ultimate test: Does the PINN learn physically consistent derivatives?

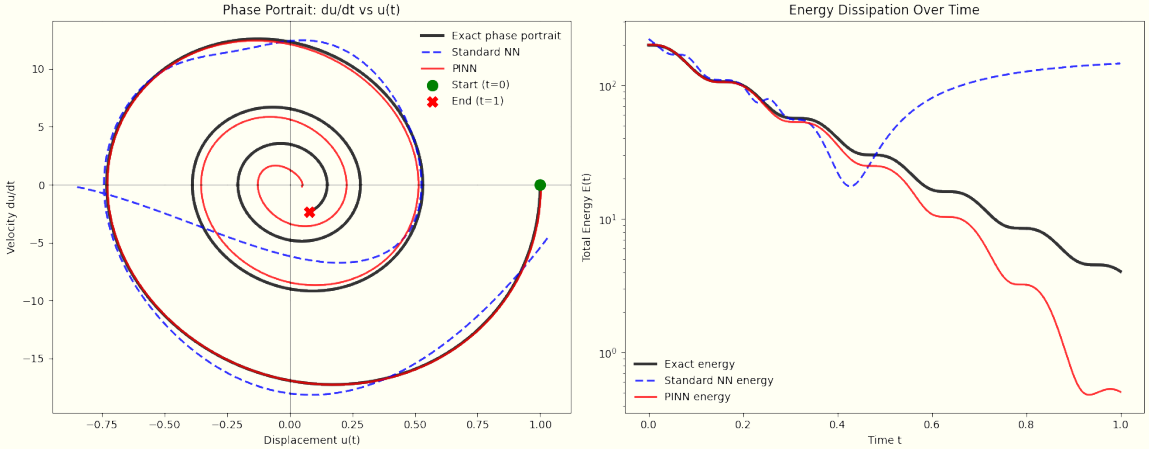


Derivative plots.

Result: The PINN learns the correct velocity (du/dt) and acceleration (d^2u/dt^2).

Deep Dive: Derivative and Phase Portrait Analysis

The ultimate test: Does the PINN learn physically consistent derivatives?



Phase portrait plots.

Outline

The 1D Poisson Problem

We now tackle a boundary value problem, the 1D Poisson equation:

$$\frac{d^2u}{dx^2} + \pi \sin(\pi x) = 0, \quad \text{for } x \in [0, 1]$$

with Dirichlet boundary conditions (BCs):

$$u(0) = 0 \quad \text{and} \quad u(1) = 0$$

Goal: Train a PINN to find the solution using only the governing equation and its BCs.

▸ Open Notebook: 1D Poisson

Method 1: Soft Constraints

Treat the boundary conditions as another component of the loss function.

Total Loss:

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{PDE}} + \lambda_{BC}\mathcal{L}_{BC}$$

Boundary Loss

A mean squared error term that penalizes violations of the BCs.

$$\mathcal{L}_{BC} = \frac{1}{N_{BC}} \sum_{i=1}^{N_{BC}} |\hat{u}_\theta(x_i) - u_{BC}|^2$$

Pros & Cons

+ **Flexible:** Easy to implement for any type of BC (Dirichlet, Neumann, etc.).
- **Approximate:** Satisfaction is not guaranteed, only encouraged.
- **Tuning:** Requires careful tuning of the weight λ_{BC}.

Method 2: Hard Constraints

Modify the network architecture to satisfy the BCs *by construction*.
For our problem with $u(0) = 0$ and $u(1) = 0$, we can define a trial solution $\tilde{u}(x)$:

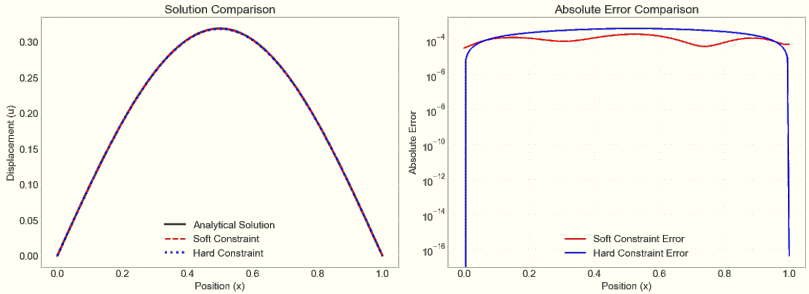
$$\tilde{u}(x) = \underbrace{x(1-x)}_{D(x)} \cdot \underbrace{\text{NN}(x;\theta)}_{\text{Network Output}}$$

The distance function $D(x)$ is zero at the boundaries, forcing $\tilde{u}(x)$ to be zero there, regardless of the network's output.

Pros & Cons

+ **Exact:** BCs are satisfied perfectly.
+ **Simpler Loss:** No need for $\mathcal{L}_{BC}$ or λ_{BC}, leading to more stable training.
- **Inflexible:** Requires designing a specific trial function for the problem's geometry and BCs, which can be difficult for complex cases.

Comparison: Soft vs. Hard Constraints



Conclusion:

- Both methods achieve high accuracy.
- The hard constraint method shows slightly lower error and, by design, has zero error at the boundaries.
- For simple geometries and Dirichlet BCs, **hard constraints are often superior**.
- For complex problems, **soft constraints offer greater versatility**.

Outline

Forward vs. Inverse Problems

Forward Problem

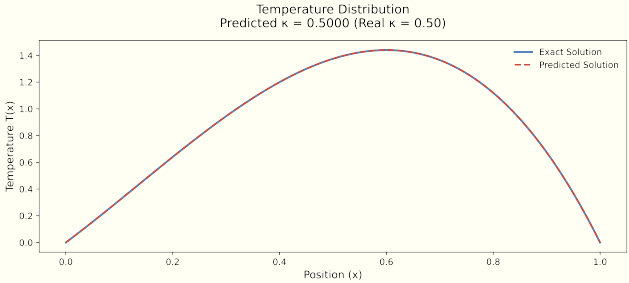
- **Given:** Full physical model (equations + parameters).
- **Find:** The solution $u(x, t)$.
- *Example: Simulate temperature given thermal conductivity.*

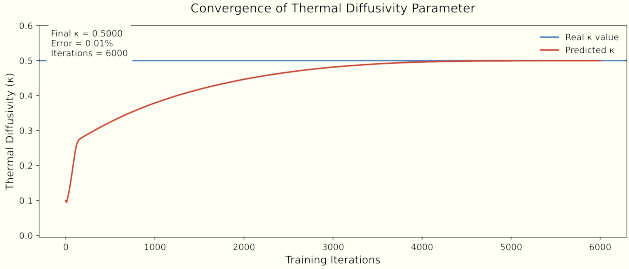
Inverse Problem

- **Given:** Sparse measurements of the solution $u(x, t)$.
- **Find:** Unknown physical parameters in the model.
- *Example: Infer thermal conductivity from temperature measurements.*

Open Notebook: Inverse Heat

Forward vs. Inverse Problems





The PINN Approach to Inverse Problems

The Key Insight: Treat the unknown physical parameters as additional trainable variables in the network.

Problem: 1D steady-state heat conduction.

$$-k\frac{d^2T}{dx^2} = f(x)$$

Here, the thermal diffusivity k is **unknown**.

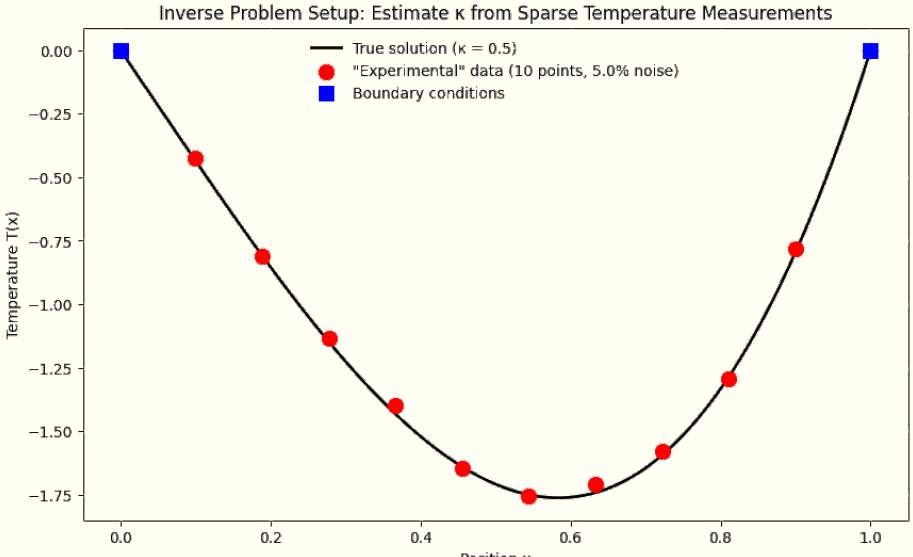
PINN Framework:

- The neural network learns the temperature field: $\hat{T}_\theta(x)$.
- A new trainable parameter is introduced: $\hat{k}$.
- The optimizer updates both the network weights θ and the parameter $\hat{k}$ simultaneously.

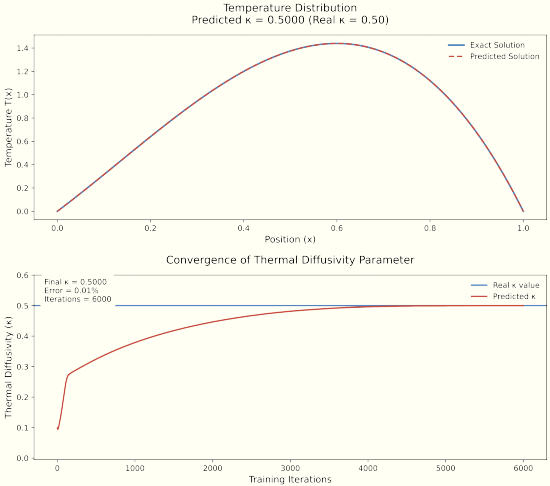
Loss Function: $\mathcal{L}(\theta, \hat{k}) = \mathcal{L}_{\text{data}} + \mathcal{L}_{\text{PDE}} + \mathcal{L}_{\text{BC}}$ where the physics loss now includes the trainable parameter $\hat{k}$:

$$\mathcal{L}_{\text{PDE}} = \frac{1}{N_f}\sum \left| -\hat{k}\frac{d^2\hat{T}_\theta}{dx^2}(x_j) - f(x_j) \right|^2$$

Implementation: Parameter Estimation



Results: Parameter Recovery



Parameter convergence and temperature field

- The estimated parameter $\hat{k}$ converges to the true value.
- The PINN simultaneously reconstructs the full, continuous temperature field accurately.
- This is achieved from very sparse and noisy data, showcasing the regularizing effect of the physics loss.

Summary: Why PINNs are Powerful

1. **Regularization Effect:**
   - Physics constraints prevent overfitting and guide the solution in data-sparse regions.
2. **Data Efficiency:**
   - Physics provides a strong inductive bias, allowing PINNs to learn from very few measurements.
3. **Accurate Derivatives:**
   - Automatic differentiation provides exact derivatives, which are learned correctly as a consequence of enforcing the physics.
4. **Versatility:**
   - The same framework can solve forward problems, inverse problems, and handle various boundary conditions.

PINNs = Universal Function Approx. + Physics Constraints + Auto. Diff.

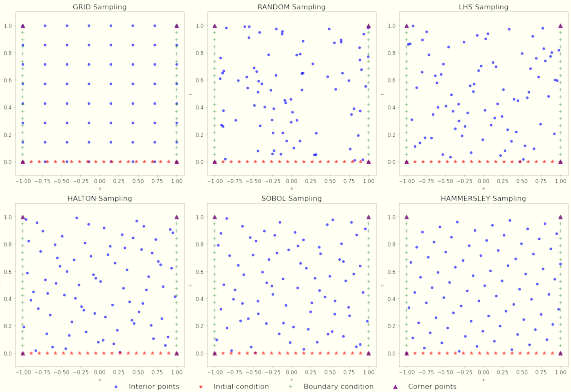
Outline

Collocation Points: Where to Enforce Physics

What are collocation points?

- Points where we evaluate PDE residual
- Do not need measurement data
- Distributed throughout domain
- More points $\rightarrow$ better physics enforcement

Key question: How should we distribute these points for optimal performance?



Different collocation sampling strategies

Collocation Sampling Strategies

Uniform Grid:

- Simple to implement
- Good coverage
- Curse of dimensionality

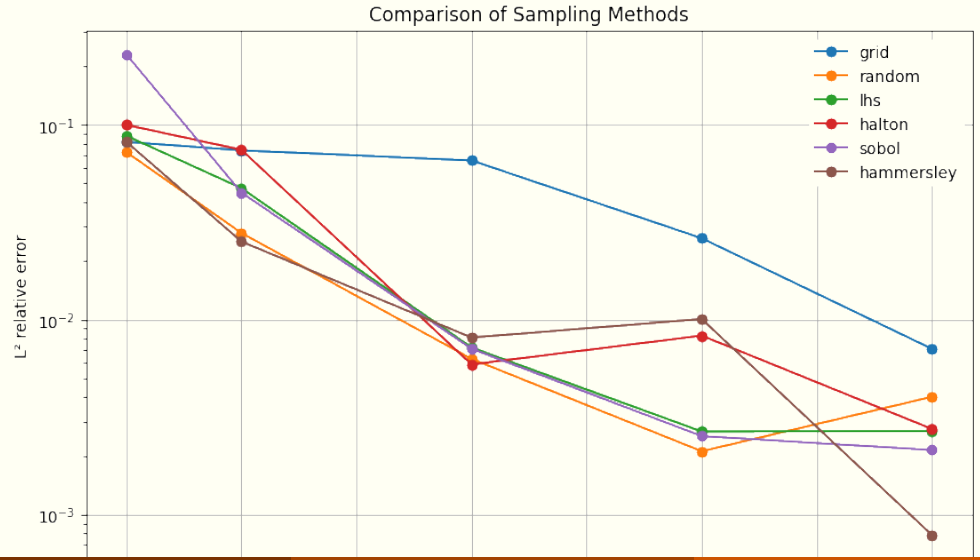
Random (Monte Carlo):

- Dimension-independent
- May cluster/leave gaps
- Easy to add points

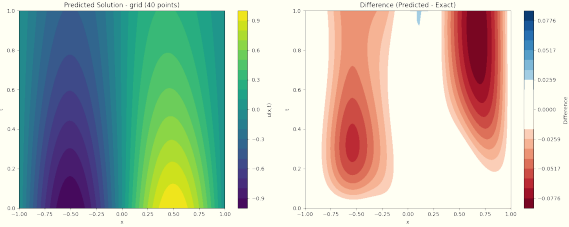
Quasi-Random:

- Better coverage than random
- Low discrepancy sequences
- Hammersley, Sobol, Halton

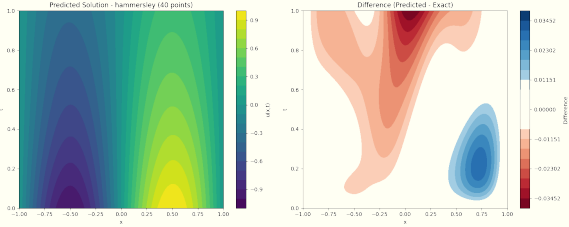
Collocation Sampling Strategies



Impact of Collocation Strategy



Error with uniform grid sampling



Error with Hammersley sampling

Observations:

- Quasi-random sampling often outperforms uniform/random
- Better space-filling properties lead to lower errors
- Particularly important in higher dimensions

Outline

The Loss Balancing Challenge

The Problem

Different loss terms can have vastly different magnitudes and gradients

Total PINN loss:

$$\mathcal{L} = \mathcal{L}_{\text{data}} + \lambda_{\text{PDE}}\mathcal{L}_{\text{PDE}} + \lambda_{\text{BC}}\mathcal{L}_{\text{BC}} + \lambda_{\text{IC}}\mathcal{L}_{\text{IC}}$$

Challenges:

- Data loss: Often $O(10^{-3})$ to $O(10^{-1})$
- PDE residual: Can be $O(10^{2})$ to $O(10^{4})$ initially
- Boundary conditions: Variable scale
- Poor balance $\rightarrow$ training instability or failure

Question: How to choose λ values optimally?

Gradient-Based Adaptive Weighting

Key idea: Balance the gradients of different loss terms

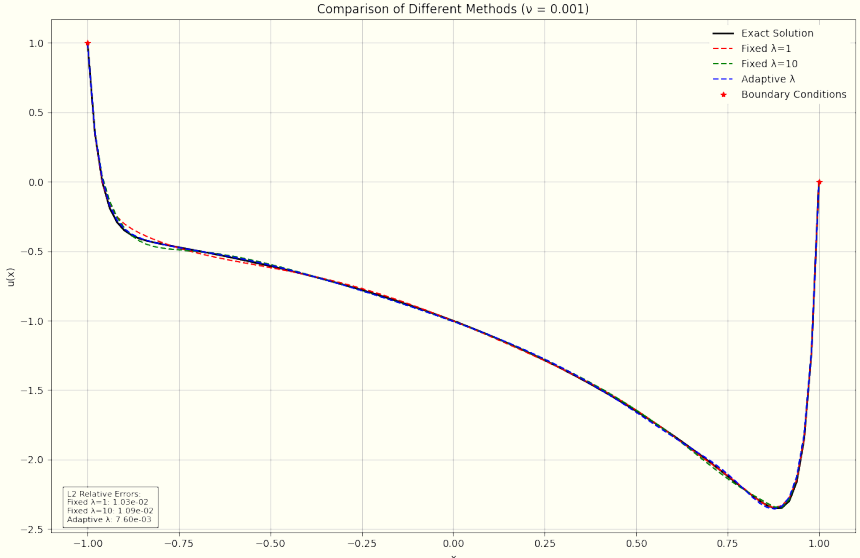
Algorithm (Wang et al., 2021):

1. Compute gradient statistics:
$$\bar{g}_i = \frac{1}{|\theta|} \sum_{\theta} |\nabla_\theta \mathcal{L}_i|$$
2. Update weights to balance gradients:
$$\lambda_i^{(k+1)} = \lambda_i^{(k)} \cdot \left(\frac{\max_j \bar{g}_j}{\bar{g}_i} \right)^{\alpha}$$
3. Apply exponential moving average for stability

Benefits:

- Prevents gradient imbalance
- Improves convergence speed
- Reduces manual tuning

Adaptive Weights in Action



Outline

The Burgers Equation: A Nonlinear PDE Challenge

Viscous Burgers equation:

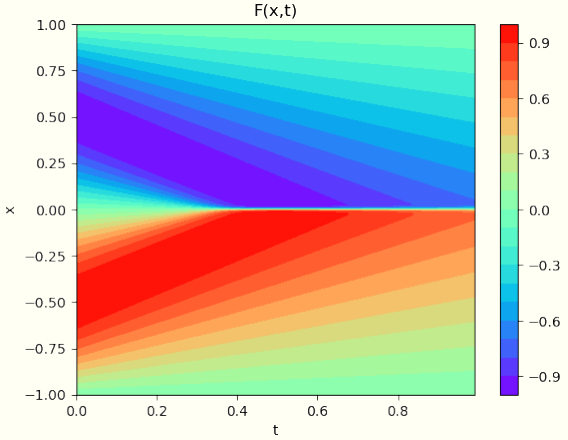
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}$$

Domain: $(x, t) \in [-1, 1] \times [0, 1]$
Initial condition:

$$u(x, 0) = -\sin(\pi x)$$

Boundary conditions:

$$u(-1, t) = u(1, t) = 0$$



Burgers equation solution showing shock formation

PINN for Burgers Equation

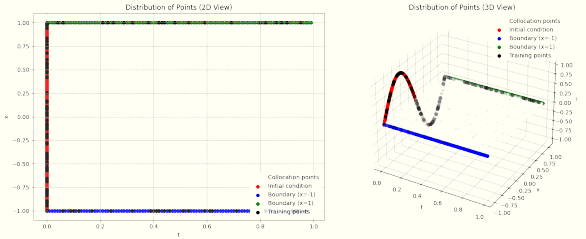
Network architecture:

- Input: (x, t)
- Output: $u(x, t)$
- Hidden layers: 8×20 neurons
- Activation: Tanh

Loss function:

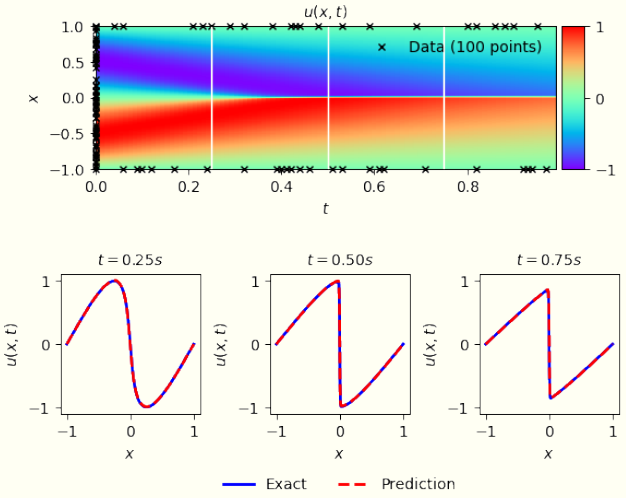
$$\mathcal{L} = \mathcal{L}_{\text{PDE}} + \mathcal{L}_{\text{IC}} + \mathcal{L}_{\text{BC}}$$

$$\mathcal{L}_{\text{PDE}} = \frac{1}{N_f} \sum \left| \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} \right|^2$$



Collocation points for Burgers equation

Burgers Equation: Forward Problem Results



Performance metrics:

- Relative L^2 error: $< 1\%$
- Training time: 5 minutes on GPU
- No mesh required
- Captures shock accurately

Inverse Problem: Parameter Discovery in Burgers

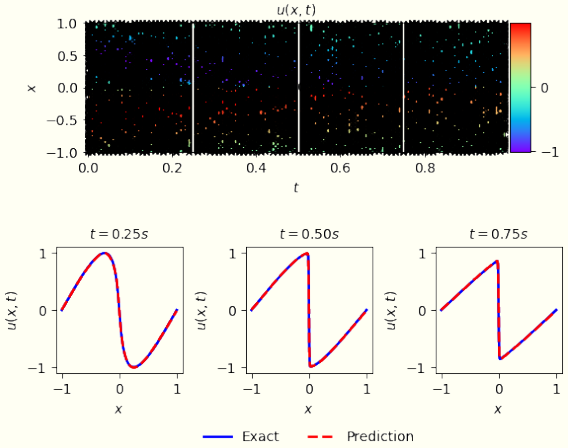
Problem setup:

- Unknown viscosity ν
- Sparse measurements of $u(x, t)$
- Goal: Recover ν and full solution

Modified loss:

$$\mathcal{L} = \mathcal{L}_{\text{data}} + \lambda \mathcal{L}_{\text{PDE}}(\nu)$$

where ν is a trainable parameter



Inverse problem: recovering solution from sparse data

Outline

Implementation Best Practices

Architecture design:

- Start with 4-8 layers, 20-50 neurons
- Tanh or Swish for smooth problems
- Adaptive activation functions for shocks
- Skip connections for deep networks

Training strategies:

- Adam optimizer with learning rate decay
- Start with $\lambda = 1$, then adapt
- Quasi-random collocation points
- Mini-batching for large problems

Common pitfalls:

- Imbalanced loss terms
- Too few collocation points
- Wrong activation for problem type
- Ignoring boundary conditions

Debugging tips:

- Visualize loss components separately
- Check gradient flow
- Start with manufactured solutions
- Verify BC/IC satisfaction

When to Use PINNs

PINNs excel at:

- Inverse problems
- Data assimilation
- High-dimensional PDEs
- Irregular geometries
- Parameter discovery
- Uncertainty quantification

Consider alternatives when:

- Need guaranteed accuracy
- Have simple, regular geometry
- Require real-time solutions
- Conservation is critical
- Problem is well-suited to FEM/FDM

PINNs complement, not replace, traditional methods

Questions?

Thank you!

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